

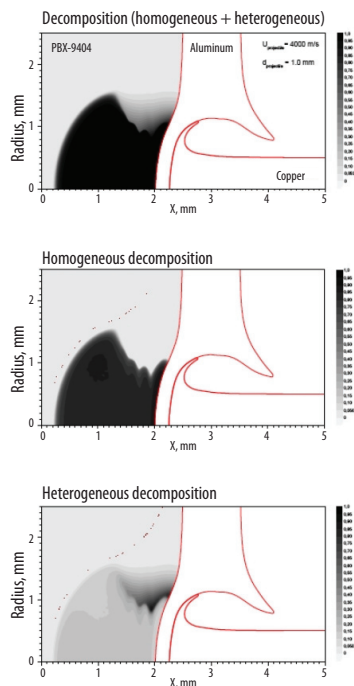
Development of an Improved Detonation Model

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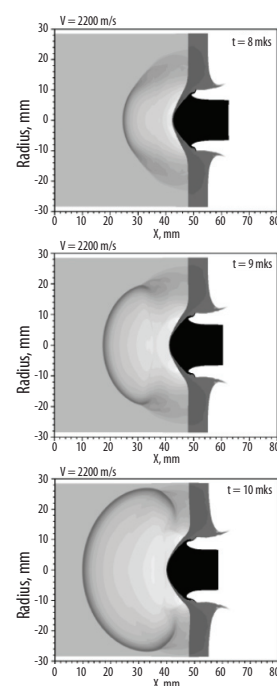
Project Description

The formulation of mathematical models capable of predicting the process of detonation of high explosives (HEs) is an area of active research. Analysis of recent experiments shows that HE decomposition occurs as the result of a complex mix of a number of fundamental decomposition mechanisms, each of which has its own domain of domination. The hot spot mechanism (heterogeneous mechanism) dominates in the pressure range from 30 kbar to 200 kbar. The homogeneous mechanism dominates at pressures > 300 kbar. In the intermediate region, 200–300 kbar, we have mixture of heterogeneous and homogeneous mechanisms. At very low pressures, $P < 20$ kbar, decomposition is governed by the so-called dislocation mechanism. It is necessary to emphasize that the stated values of boundary pressures — 30, 200 and 300 kbar — are qualitative and have concrete values for each explosive.

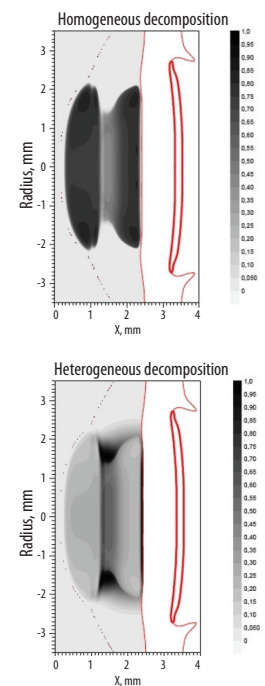
The primary goal of this project is to develop an improved model of detonation, one with accuracy on the order of 10% (existing models are considerably less accurate). The model will be applicable to standard PBX explosives and will be calibrated for PBX-9501 and PBX-9502.



Initiation of detonation in PBX 9404 shielded by aluminum for the impact of a copper rod traveling at 4000 m/s.



Initiation of detonation in Comp-B shielded by aluminum from the impact of a steel bullet traveling at 2200 m/s.



Initiation of detonation in PBX-9404 shielded by aluminum from the impact of a steel plate traveling at 1600 m/s.

The task will be performed in two stages. In the first stage (first year), it is planned to develop a numerical model with hot spot and homogeneous mechanisms of HE decomposition. This heterogeneous-homogeneous model (HH model) will be ready for precise calculations at pressures >20 kbar. In the second stage (second year), dislocation mechanisms will be incorporated into the HH model. The resultant heterogeneous-homogeneous-dislocation model (HHD model) will enable precise calculations at any pressure.

Technical Purpose and Benefits

The development of better predictive capability is essential if LANL is to meet its obligations to NNSA and the country. Models that more accurately predict

the decomposition of high explosives are of critical importance to the NNSA and LANL. Under this project, a significant improvement in predictive capability may be made possible with the development of an HHD model for HE decomposition. Considerable progress has already been made, and preliminary results look quite promising. This work supports the objectives of the NNSA and both research institutions (LANL and RAS Inst. of Chemical Physics) as they endeavor to improve their predictive capabilities in the area of HE detonation.

Collaboration between Los Alamos National Laboratory, Los Alamos, NM, USA, and the Institute of Chemical Physics – Russian Academy of Science, Moscow, Russia

